



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 12:45 PM BST

PDB ID : 4DJ8
Title : Structure of the hemagglutinin complexed with 6SLN from a highly pathogenic H7N7 influenza virus
Authors : Yang, H.; Carney, P.J.; Donis, R.O.; Stevens, J.
Deposited on : 2012-02-01
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

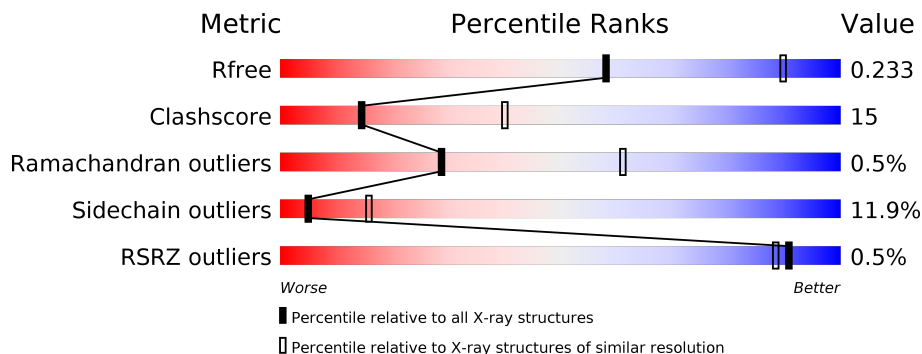
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	327	
1	C	327	
1	E	327	
2	B	177	
2	D	177	
2	F	177	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11749 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	316	Total 2422	C 1502	N 435	O 471	S 14	4	0	0
1	C	316	Total 2422	C 1502	N 435	O 471	S 14	4	0	0
1	E	317	Total 2437	C 1510	N 440	O 473	S 14	3	1	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	ALA	-	expression tag	UNP Q6VMK1
A	-2	ASP	-	expression tag	UNP Q6VMK1
A	-1	PRO	-	expression tag	UNP Q6VMK1
A	0	GLY	-	expression tag	UNP Q6VMK1
C	-3	ALA	-	expression tag	UNP Q6VMK1
C	-2	ASP	-	expression tag	UNP Q6VMK1
C	-1	PRO	-	expression tag	UNP Q6VMK1
C	0	GLY	-	expression tag	UNP Q6VMK1
E	-3	ALA	-	expression tag	UNP Q6VMK1
E	-2	ASP	-	expression tag	UNP Q6VMK1
E	-1	PRO	-	expression tag	UNP Q6VMK1
E	0	GLY	-	expression tag	UNP Q6VMK1

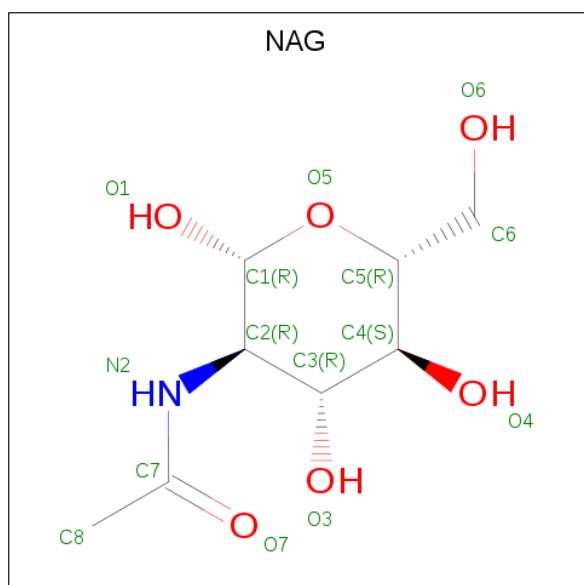
- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	170	Total 1380	C 851	N 243	O 279	S 7	4	0	0
2	D	171	Total 1388	C 857	N 244	O 280	S 7	0	0	0
2	F	169	Total 1369	C 845	N 239	O 278	S 7	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP Q6VMK1
B	176	GLY	-	expression tag	UNP Q6VMK1
B	177	ARG	-	expression tag	UNP Q6VMK1
D	175	SER	-	expression tag	UNP Q6VMK1
D	176	GLY	-	expression tag	UNP Q6VMK1
D	177	ARG	-	expression tag	UNP Q6VMK1
F	175	SER	-	expression tag	UNP Q6VMK1
F	176	GLY	-	expression tag	UNP Q6VMK1
F	177	ARG	-	expression tag	UNP Q6VMK1

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



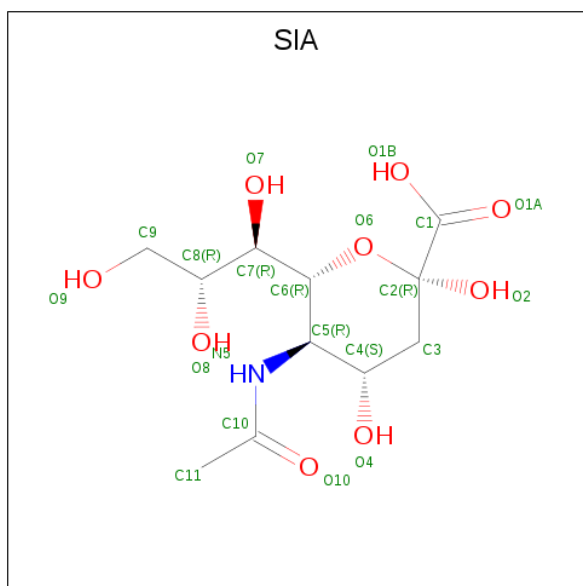
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is N-acetyl-alpha-neuraminic acid (three-letter code: SIA) (formula: C₁₁H₁₉NO₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			20	11	1	8		
4	C	1	Total	C	N	O	0	0
			20	11	1	8		
4	E	1	Total	C	N	O	0	0
			20	11	1	8		

- Molecule 5 is water.

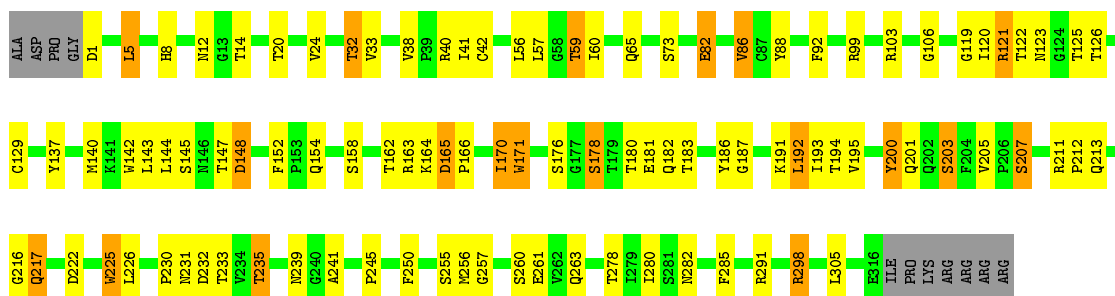
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total 22	O 22	0	0
5	B	14	Total 14	O 14	0	0
5	C	25	Total 25	O 25	0	0
5	D	11	Total 11	O 11	0	0
5	E	18	Total 18	O 18	0	0
5	F	13	Total 13	O 13	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

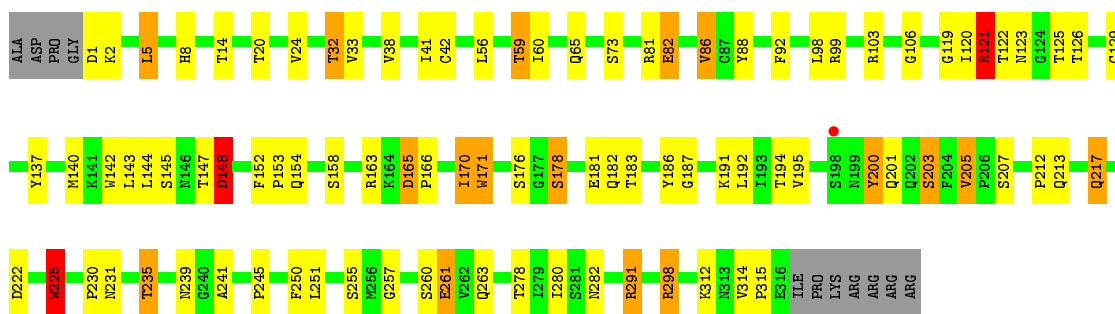
- Molecule 1: Hemagglutinin

Chain A: 



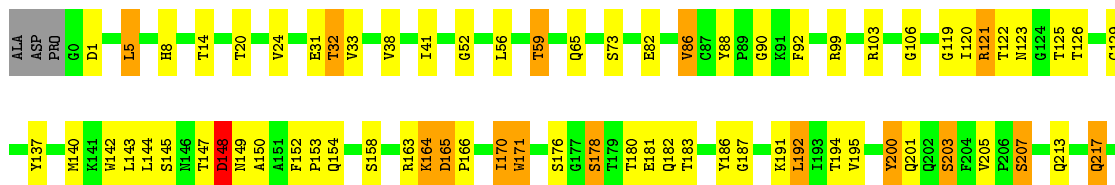
- Molecule 1: Hemagglutinin

Chain C: 



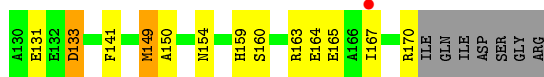
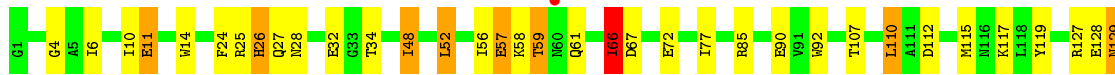
- Molecule 1: Hemagglutinin

Chain E: 

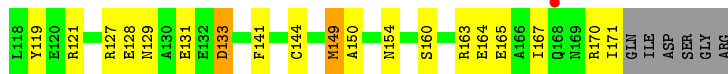
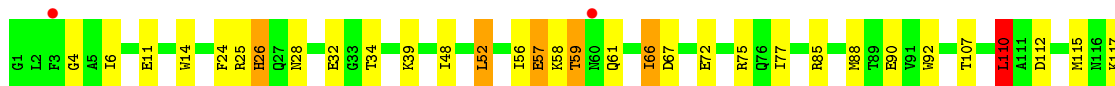




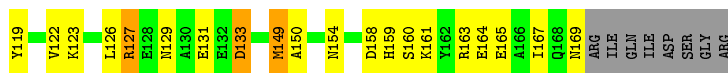
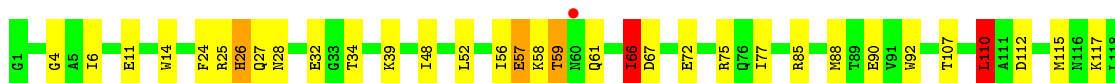
• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



• Molecule 2: Hemagglutinin



4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	203.77Å 117.60Å 120.46Å 90.00° 124.15° 90.00°	Depositor
Resolution (Å)	48.23 – 2.80 48.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.23-2.80) 99.2 (48.23-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.190 , 0.235 0.189 , 0.233	Depositor DCC
R_{free} test set	2934 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 27.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.001 for $-1/2^*h-3/2^*k-l, -1/2^*h+1/2^*k-l, 1/2^*h+1/2^*k$ 0.000 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-l$ 0.010 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-l$ 0.003 for $-1/2^*h+3/2^*k-l, 1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k$ 0.000 for $-h-k-l, l, k$ 0.013 for $-h+k-l, -l, -k$ 0.000 for $-1/2^*h-1/2^*k+l, -1/2^*h-1/2^*k-l, 1/2^*h-1/2^*k$ 0.012 for $-1/2^*h+1/2^*k+l, 1/2^*h-1/2^*k+l, 1/2^*h+1/2^*k$ 0.438 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-l$ 0.448 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-l$ 0.010 for $-h-2^*l, -k, l$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.91	4/2468 (0.2%)	0.93	2/3337 (0.1%)
1	C	0.99	8/2468 (0.3%)	1.04	8/3337 (0.2%)
1	E	0.96	4/2483 (0.2%)	0.93	3/3356 (0.1%)
2	B	0.87	1/1404 (0.1%)	0.85	1/1892 (0.1%)
2	D	0.87	1/1412 (0.1%)	0.86	1/1903 (0.1%)
2	F	0.90	1/1393 (0.1%)	0.84	1/1878 (0.1%)
All	All	0.93	19/11628 (0.2%)	0.93	16/15703 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	F	0	1
All	All	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	164	LYS	CG-CD	-11.97	1.11	1.52
1	C	148	ASP	CA-CB	-10.29	1.31	1.53
1	C	225	TRP	CD2-CE2	10.07	1.53	1.41
1	C	148	ASP	CB-CG	7.50	1.67	1.51
1	E	171	TRP	CD2-CE2	7.07	1.49	1.41
1	C	171	TRP	CD2-CE2	6.97	1.49	1.41
1	E	225	TRP	NE1-CE2	-6.52	1.29	1.37
1	A	225	TRP	NE1-CE2	-6.39	1.29	1.37
1	C	2	LYS	CG-CD	-6.20	1.31	1.52
2	B	14	TRP	CD2-CE2	6.00	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	225	TRP	CD2-CE3	-5.69	1.31	1.40
1	A	171	TRP	CD2-CE2	5.66	1.48	1.41
2	F	14	TRP	CD2-CE2	5.59	1.48	1.41
1	C	225	TRP	CD1-NE1	-5.58	1.28	1.38
1	A	142	TRP	CD2-CE2	5.45	1.47	1.41
2	D	14	TRP	CD2-CE2	5.42	1.47	1.41
1	E	142	TRP	CD2-CE2	5.32	1.47	1.41
1	A	129	CYS	CB-SG	-5.23	1.73	1.81
1	C	142	TRP	CD2-CE2	5.09	1.47	1.41

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	148	ASP	CB-CG-OD2	-15.69	104.18	118.30
1	C	225	TRP	CE2-CD2-CG	-12.13	97.60	107.30
1	C	148	ASP	CB-CG-OD1	12.03	129.13	118.30
1	C	225	TRP	CG-CD2-CE3	8.81	141.83	133.90
1	E	148	ASP	C-N-CA	7.57	140.62	121.70
1	C	225	TRP	CA-CB-CG	-6.59	101.18	113.70
1	C	225	TRP	CB-CG-CD1	-6.09	119.08	127.00
1	E	164	LYS	CB-CG-CD	6.00	127.19	111.60
2	B	110	LEU	CA-CB-CG	5.94	128.96	115.30
2	D	110	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	40	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	F	110	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	256	MET	CA-CB-CG	5.07	121.92	113.30
1	E	256	MET	CA-CB-CG	5.04	121.87	113.30
1	C	148	ASP	CB-CA-C	-5.03	100.35	110.40
1	C	121	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	66	ILE	Peptide
2	F	66	ILE	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2422	0	2369	80	0
1	C	2422	0	2369	81	0
1	E	2437	0	2384	72	0
2	B	1380	0	1283	54	0
2	D	1388	0	1294	51	0
2	F	1369	0	1270	52	0
3	A	42	0	39	0	0
3	B	14	0	13	0	0
3	C	42	0	39	0	0
3	D	14	0	13	2	0
3	E	42	0	39	0	0
3	F	14	0	13	2	0
4	A	20	0	17	0	0
4	C	20	0	17	0	0
4	E	20	0	17	0	0
5	A	22	0	0	3	0
5	B	14	0	0	1	0
5	C	25	0	0	4	0
5	D	11	0	0	1	0
5	E	18	0	0	0	0
5	F	13	0	0	3	0
All	All	11749	0	11176	351	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (351) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:98:LEU:HD13	1:C:225:TRP:CE3	1.79	1.17
1:C:98:LEU:HD13	1:C:225:TRP:HE3	1.13	1.07
2:B:165:GLU:HG2	5:B:313:HOH:O	1.59	1.02
2:B:59:THR:HG23	2:B:61:GLN:H	1.21	1.02
1:C:225:TRP:O	1:C:225:TRP:CD1	2.12	1.01
2:D:59:THR:HG23	2:D:61:GLN:H	1.23	1.00
2:F:59:THR:HG23	2:F:61:GLN:H	1.24	0.99
1:E:120:ILE:HG22	1:E:121:ARG:N	1.83	0.92
2:F:165:GLU:HG2	5:F:310:HOH:O	1.68	0.92
1:A:5:LEU:H	1:A:5:LEU:HD22	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ARG:HE	2:B:34:THR:CG2	1.82	0.92
1:E:5:LEU:HD22	1:E:5:LEU:H	1.34	0.92
1:C:5:LEU:HD22	1:C:5:LEU:H	1.32	0.91
1:E:120:ILE:HG22	1:E:121:ARG:H	1.36	0.91
1:C:225:TRP:C	1:C:225:TRP:CD1	2.39	0.91
1:C:120:ILE:HG22	1:C:121:ARG:N	1.86	0.91
1:A:120:ILE:HG22	1:A:121:ARG:N	1.85	0.89
2:D:25:ARG:HE	2:D:34:THR:CG2	1.86	0.87
2:B:57:GLU:HG2	2:B:58:LYS:H	1.40	0.86
2:F:25:ARG:HE	2:F:34:THR:CG2	1.88	0.86
2:B:66:ILE:HD12	2:B:66:ILE:H	1.40	0.86
2:B:25:ARG:HE	2:B:34:THR:HG22	1.38	0.85
2:D:57:GLU:HG2	2:D:58:LYS:H	1.41	0.85
1:E:121:ARG:HH11	1:E:121:ARG:HG3	1.41	0.85
2:F:25:ARG:HE	2:F:34:THR:HG22	1.40	0.84
2:D:25:ARG:HE	2:D:34:THR:HG22	1.40	0.84
2:F:66:ILE:HD12	2:F:66:ILE:H	1.42	0.84
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.44	0.83
2:F:57:GLU:HG2	2:F:58:LYS:H	1.44	0.82
2:D:66:ILE:H	2:D:66:ILE:HD12	1.43	0.82
1:A:120:ILE:HG22	1:A:121:ARG:H	1.40	0.81
1:A:183:THR:HA	1:A:187:GLY:O	1.81	0.80
1:C:120:ILE:HG22	1:C:121:ARG:H	1.42	0.80
1:C:183:THR:HA	1:C:187:GLY:O	1.81	0.80
1:A:120:ILE:CG2	1:A:144:LEU:O	2.31	0.79
1:E:183:THR:HA	1:E:187:GLY:O	1.82	0.79
1:E:120:ILE:CG2	1:E:144:LEU:O	2.31	0.78
1:C:120:ILE:CG2	1:C:144:LEU:O	2.33	0.77
2:D:59:THR:CG2	2:D:61:GLN:H	1.98	0.77
1:A:82:GLU:OE2	5:A:507:HOH:O	2.03	0.75
1:C:121:ARG:HH11	1:C:121:ARG:HG3	1.49	0.75
1:C:92:PHE:HE2	1:C:170:ILE:HD11	1.50	0.75
1:C:98:LEU:CD1	1:C:225:TRP:HE3	1.97	0.75
3:F:201:NAG:H83	5:F:305:HOH:O	1.85	0.75
1:A:120:ILE:HG21	1:A:144:LEU:O	1.88	0.74
1:E:120:ILE:HG21	1:E:144:LEU:O	1.86	0.74
2:D:163:ARG:O	2:D:167:ILE:HG13	1.88	0.74
3:D:201:NAG:H83	5:D:305:HOH:O	1.87	0.73
1:C:178:SER:HB2	1:C:181:GLU:H	1.53	0.72
2:B:59:THR:CG2	2:B:61:GLN:H	1.99	0.72
1:C:120:ILE:HG21	1:C:144:LEU:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:121:ARG:HH11	1:E:121:ARG:CG	2.04	0.71
2:B:128:GLU:OE2	2:B:170:ARG:NH1	2.23	0.70
2:B:163:ARG:O	2:B:167:ILE:HG13	1.90	0.70
1:E:92:PHE:HE2	1:E:170:ILE:HD11	1.55	0.70
1:C:38:VAL:HG21	1:C:280:ILE:HD12	1.71	0.70
1:A:92:PHE:HE2	1:A:170:ILE:HD11	1.54	0.70
1:C:98:LEU:HD13	1:C:225:TRP:CZ3	2.27	0.70
2:B:6:ILE:HD12	2:B:112:ASP:HA	1.73	0.70
2:F:59:THR:CG2	2:F:61:GLN:H	2.02	0.69
2:F:59:THR:HG23	2:F:61:GLN:N	2.05	0.69
1:A:38:VAL:HG21	1:A:280:ILE:HD12	1.76	0.68
2:D:59:THR:HG23	2:D:61:GLN:N	2.05	0.68
1:E:178:SER:HB2	1:E:181:GLU:H	1.58	0.68
2:B:59:THR:HG23	2:B:61:GLN:N	2.04	0.68
2:F:25:ARG:HH21	2:F:34:THR:HG21	1.59	0.67
2:D:25:ARG:HH21	2:D:34:THR:HG21	1.58	0.67
1:C:1:ASP:OD2	5:C:514:HOH:O	2.11	0.67
1:C:225:TRP:H	1:C:225:TRP:HD1	1.41	0.67
2:D:57:GLU:HG2	2:D:58:LYS:N	2.10	0.67
1:C:82:GLU:OE2	5:C:522:HOH:O	2.12	0.67
2:F:66:ILE:N	2:F:66:ILE:HD12	2.07	0.67
2:B:57:GLU:HG2	2:B:58:LYS:N	2.10	0.67
1:A:178:SER:HB2	1:A:181:GLU:H	1.59	0.67
2:B:25:ARG:HE	2:B:34:THR:HG21	1.59	0.67
2:F:163:ARG:O	2:F:167:ILE:HG13	1.94	0.67
1:C:201:GLN:NE2	1:E:222:ASP:OD1	2.23	0.66
1:A:201:GLN:NE2	1:C:222:ASP:OD1	2.24	0.66
1:A:121:ARG:NH1	1:A:145:SER:O	2.26	0.65
1:A:121:ARG:HH11	1:A:121:ARG:CG	2.08	0.65
1:E:120:ILE:CG2	1:E:121:ARG:N	2.57	0.65
2:F:164:GLU:HG3	2:F:165:GLU:N	2.12	0.65
2:F:164:GLU:HG3	2:F:165:GLU:H	1.62	0.65
2:B:25:ARG:HH21	2:B:34:THR:HG21	1.60	0.65
1:A:120:ILE:CG2	1:A:121:ARG:N	2.60	0.64
1:A:140:MET:HE2	1:A:245:PRO:HA	1.78	0.64
1:C:140:MET:HE2	1:C:245:PRO:HA	1.79	0.64
1:E:140:MET:HE2	1:E:245:PRO:HA	1.79	0.64
1:C:98:LEU:CD1	1:C:225:TRP:CE3	2.70	0.64
1:C:154:GLN:OE1	1:C:239:ASN:HB3	1.97	0.63
1:E:38:VAL:HG21	1:E:280:ILE:HD12	1.79	0.63
1:A:282:ASN:HB3	2:B:56:ILE:HG23	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:128:GLU:OE2	2:D:170:ARG:NH1	2.29	0.63
1:C:298:ARG:HG2	2:D:92:TRP:CD2	2.34	0.63
1:E:154:GLN:OE1	1:E:239:ASN:HB3	1.99	0.63
2:D:117:LYS:HE3	2:F:4:GLY:HA2	1.80	0.63
1:A:88:TYR:CE1	1:A:217:GLN:HG2	2.33	0.63
2:D:164:GLU:HG3	2:D:165:GLU:N	2.14	0.63
2:F:57:GLU:HG2	2:F:58:LYS:N	2.12	0.63
1:C:121:ARG:HH11	1:C:121:ARG:CG	2.11	0.63
1:C:121:ARG:NH1	1:C:145:SER:O	2.31	0.62
1:C:88:TYR:CE1	1:C:217:GLN:HG2	2.35	0.62
2:B:4:GLY:HA2	2:F:117:LYS:HE3	1.82	0.62
1:C:291:ARG:NH1	2:D:67:ASP:HB3	2.13	0.62
2:B:117:LYS:HE3	2:D:4:GLY:HA2	1.80	0.62
2:D:66:ILE:HD12	2:D:66:ILE:N	2.10	0.62
1:A:154:GLN:OE1	1:A:239:ASN:HB3	2.00	0.62
2:B:141:PHE:CD1	2:B:170:ARG:HG2	2.35	0.62
2:D:25:ARG:HE	2:D:34:THR:HG21	1.65	0.62
2:B:164:GLU:HG3	2:B:165:GLU:N	2.14	0.62
1:C:291:ARG:HD2	2:D:67:ASP:OD2	2.00	0.62
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.14	0.61
1:E:88:TYR:CE1	1:E:217:GLN:HG2	2.35	0.61
1:A:298:ARG:HG2	2:B:92:TRP:CD2	2.35	0.60
2:B:160:SER:HA	2:B:163:ARG:HB2	1.81	0.60
1:C:225:TRP:O	1:C:225:TRP:HD1	1.76	0.60
1:C:225:TRP:N	1:C:225:TRP:HD1	1.97	0.60
2:D:164:GLU:HG3	2:D:165:GLU:H	1.67	0.60
1:C:225:TRP:N	1:C:225:TRP:CD1	2.65	0.59
2:F:160:SER:HA	2:F:163:ARG:HB2	1.82	0.59
1:E:282:ASN:HB3	2:F:56:ILE:HG23	1.84	0.59
1:A:119:GLY:C	1:A:120:ILE:HG13	2.22	0.59
1:A:291:ARG:NH1	2:B:67:ASP:HB3	2.17	0.59
1:E:121:ARG:HG3	1:E:121:ARG:NH1	2.11	0.59
1:A:170:ILE:HD12	1:A:225:TRP:HB3	1.83	0.59
2:B:66:ILE:HD12	2:B:66:ILE:N	2.05	0.59
1:E:120:ILE:CG2	1:E:121:ARG:H	2.13	0.59
1:C:119:GLY:C	1:C:120:ILE:HG13	2.23	0.58
1:A:158:SER:OG	1:A:235:THR:HB	2.03	0.58
1:A:140:MET:CE	1:A:245:PRO:HA	2.33	0.58
1:C:147:THR:CG2	1:C:148:ASP:N	2.67	0.58
2:D:160:SER:HA	2:D:163:ARG:HB2	1.84	0.58
1:E:298:ARG:HG2	2:F:92:TRP:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:ILE:HD12	2:F:112:ASP:HA	1.86	0.57
1:A:99:ARG:O	1:A:103:ARG:HG3	2.04	0.57
1:C:282:ASN:HB3	2:D:56:ILE:HG23	1.86	0.57
1:E:119:GLY:C	1:E:120:ILE:HG13	2.24	0.57
2:F:25:ARG:HE	2:F:34:THR:HG21	1.67	0.57
1:C:147:THR:CG2	1:C:148:ASP:H	2.17	0.57
1:A:298:ARG:NE	5:A:521:HOH:O	2.37	0.57
1:A:32:THR:HG22	1:A:33:VAL:HG23	1.86	0.57
1:C:98:LEU:HA	1:C:225:TRP:HZ3	1.70	0.57
1:E:291:ARG:HD2	2:F:67:ASP:OD2	2.05	0.56
2:D:141:PHE:CD1	2:D:170:ARG:HG2	2.40	0.56
1:E:291:ARG:NH1	2:F:67:ASP:HB3	2.20	0.56
2:D:6:ILE:HD12	2:D:112:ASP:HA	1.88	0.56
2:F:67:ASP:OD2	2:F:85:ARG:NH2	2.38	0.56
1:E:121:ARG:NH1	1:E:145:SER:O	2.35	0.56
1:E:1:ASP:HB2	2:F:28:ASN:HA	1.87	0.56
1:A:147:THR:CG2	1:A:148:ASP:N	2.69	0.56
2:B:164:GLU:HG3	2:B:165:GLU:H	1.69	0.56
1:E:170:ILE:HD12	1:E:225:TRP:HB3	1.87	0.56
1:E:41:ILE:HD11	1:E:260:SER:OG	2.06	0.56
1:C:147:THR:HG22	1:C:148:ASP:N	2.21	0.55
1:E:32:THR:HG22	1:E:33:VAL:HG23	1.88	0.55
1:C:120:ILE:CG2	1:C:121:ARG:H	2.17	0.55
1:C:203:SER:OG	1:E:207:SER:HB3	2.07	0.55
1:C:120:ILE:CG2	1:C:121:ARG:N	2.60	0.55
2:F:75:ARG:HD3	3:F:201:NAG:H81	1.89	0.55
1:C:191:LYS:HA	1:C:239:ASN:HD21	1.72	0.55
1:C:121:ARG:NH1	1:C:121:ARG:HG3	2.19	0.54
2:D:163:ARG:NH2	2:F:131:GLU:OE1	2.37	0.54
1:A:120:ILE:CG2	1:A:121:ARG:H	2.17	0.54
1:C:298:ARG:NE	5:C:519:HOH:O	2.39	0.54
1:E:140:MET:CE	1:E:245:PRO:HA	2.37	0.54
1:A:191:LYS:O	1:A:205:VAL:HG13	2.08	0.54
1:A:291:ARG:HD2	2:B:67:ASP:OD2	2.08	0.54
1:C:140:MET:CE	1:C:245:PRO:HA	2.37	0.54
1:C:158:SER:OG	1:C:235:THR:HB	2.08	0.54
1:A:147:THR:HG22	1:A:148:ASP:N	2.23	0.54
2:B:26:HIS:HB2	2:B:149:MET:CE	2.38	0.54
1:E:120:ILE:HG23	1:E:144:LEU:O	2.07	0.53
1:C:41:ILE:HD11	1:C:260:SER:OG	2.09	0.53
1:E:191:LYS:HA	1:E:239:ASN:HD21	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:OE1	2:F:163:ARG:NH2	2.41	0.53
1:C:32:THR:HG22	1:C:33:VAL:HG23	1.91	0.53
1:A:147:THR:CG2	1:A:148:ASP:H	2.22	0.53
1:A:120:ILE:HG23	1:A:144:LEU:O	2.06	0.52
1:A:191:LYS:HA	1:A:239:ASN:HD21	1.74	0.52
1:C:191:LYS:O	1:C:205:VAL:HG13	2.09	0.52
1:A:1:ASP:HB2	2:B:28:ASN:HA	1.92	0.52
1:C:92:PHE:CE2	1:C:170:ILE:HD11	2.40	0.52
1:A:203:SER:OG	1:C:207:SER:HB3	2.09	0.52
2:D:26:HIS:HB2	2:D:149:MET:CE	2.39	0.52
2:F:26:HIS:HB2	2:F:149:MET:CE	2.40	0.52
1:E:158:SER:OG	1:E:235:THR:HB	2.09	0.52
1:E:191:LYS:O	1:E:205:VAL:HG13	2.10	0.52
1:C:120:ILE:HG23	1:C:144:LEU:O	2.06	0.51
1:C:59:THR:HG22	1:C:60:ILE:HG12	1.91	0.51
1:A:222:ASP:OD1	1:E:201:GLN:NE2	2.32	0.51
2:D:75:ARG:HD3	3:D:201:NAG:H81	1.91	0.51
1:E:56:LEU:O	1:E:59:THR:HB	2.11	0.51
1:A:41:ILE:HD11	1:A:260:SER:OG	2.11	0.51
2:B:133:ASP:C	2:B:133:ASP:OD2	2.49	0.51
1:C:213:GLN:HA	1:C:217:GLN:O	2.10	0.51
1:A:12:ASN:HB3	5:A:522:HOH:O	2.11	0.51
2:F:24:PHE:O	2:F:34:THR:HA	2.11	0.51
5:C:514:HOH:O	2:D:144:CYS:N	2.20	0.51
2:D:61:GLN:OE1	2:F:90:GLU:OE2	2.29	0.51
2:D:133:ASP:OD2	2:D:133:ASP:C	2.49	0.51
1:E:86:VAL:HG22	1:E:137:TYR:OH	2.11	0.51
1:E:5:LEU:H	1:E:5:LEU:CD2	2.17	0.50
1:C:1:ASP:HB2	2:D:28:ASN:HA	1.94	0.50
1:C:56:LEU:O	1:C:59:THR:HB	2.11	0.50
2:B:25:ARG:NH2	2:B:34:THR:HG21	2.26	0.50
1:E:225:TRP:N	1:E:225:TRP:CD1	2.79	0.50
2:B:24:PHE:O	2:B:34:THR:HA	2.13	0.49
1:E:123:ASN:O	1:E:125:THR:HG23	2.12	0.49
1:E:171:TRP:CH2	1:E:195:VAL:HG11	2.47	0.49
1:A:5:LEU:H	1:A:5:LEU:CD2	2.18	0.49
1:C:86:VAL:HG22	1:C:137:TYR:OH	2.13	0.49
2:B:56:ILE:HG22	2:B:56:ILE:O	2.13	0.49
1:C:123:ASN:O	1:C:125:THR:HG23	2.13	0.49
2:B:67:ASP:OD2	2:B:85:ARG:NH2	2.44	0.48
2:F:133:ASP:C	2:F:133:ASP:OD2	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:56:ILE:O	2:F:56:ILE:HG22	2.13	0.48
2:D:56:ILE:O	2:D:56:ILE:HG22	2.13	0.48
1:A:59:THR:HG22	1:A:60:ILE:HG12	1.96	0.48
1:C:163:ARG:HD3	1:C:250:PHE:CZ	2.49	0.48
2:D:24:PHE:O	2:D:34:THR:HA	2.14	0.48
1:A:119:GLY:O	1:A:120:ILE:HG13	2.14	0.48
1:A:152:PHE:CD2	1:A:239:ASN:C	2.88	0.48
1:A:207:SER:HB3	1:E:203:SER:OG	2.13	0.48
2:B:61:GLN:OE1	2:D:90:GLU:OE2	2.31	0.47
1:A:86:VAL:HG22	1:A:137:TYR:OH	2.14	0.47
1:A:213:GLN:HA	1:A:217:GLN:O	2.15	0.47
1:A:225:TRP:CD1	1:A:225:TRP:N	2.82	0.47
2:B:163:ARG:NH2	2:D:131:GLU:OE1	2.45	0.47
1:E:152:PHE:CD2	1:E:239:ASN:C	2.87	0.47
2:B:11:GLU:H	2:B:11:GLU:HG2	1.49	0.47
1:E:106:GLY:HA2	1:E:255:SER:HB3	1.96	0.47
1:C:103:ARG:HB3	1:C:257:GLY:HA3	1.96	0.47
2:B:61:GLN:OE1	2:D:90:GLU:HG2	2.15	0.47
2:F:25:ARG:NH2	2:F:34:THR:HG21	2.28	0.47
2:D:25:ARG:NH2	2:D:34:THR:HG21	2.26	0.47
2:D:57:GLU:CG	2:D:58:LYS:N	2.75	0.47
1:C:119:GLY:O	1:C:120:ILE:HG13	2.14	0.47
1:C:152:PHE:CD2	1:C:239:ASN:C	2.88	0.47
1:C:99:ARG:O	1:C:103:ARG:HG3	2.15	0.47
2:B:57:GLU:CG	2:B:58:LYS:N	2.74	0.46
1:A:163:ARG:HD3	1:A:250:PHE:CZ	2.50	0.46
1:C:171:TRP:CH2	1:C:195:VAL:HG11	2.50	0.46
1:E:119:GLY:O	1:E:120:ILE:HG13	2.14	0.46
2:B:150:ALA:O	2:B:154:ASN:ND2	2.49	0.46
2:B:90:GLU:OE2	2:F:61:GLN:OE1	2.34	0.46
1:A:171:TRP:CH2	1:A:195:VAL:HG11	2.51	0.46
2:B:25:ARG:NE	2:B:34:THR:HG21	2.28	0.46
1:E:149:ASN:OD1	1:E:183:THR:HG22	2.16	0.46
1:A:42:CYS:HB2	1:A:278:THR:HG21	1.98	0.46
2:F:165:GLU:CG	5:F:310:HOH:O	2.44	0.46
1:A:92:PHE:CE2	1:A:170:ILE:HD11	2.42	0.45
1:C:186:TYR:CZ	1:C:241:ALA:HA	2.51	0.45
1:E:103:ARG:HB3	1:E:257:GLY:HA3	1.97	0.45
1:A:200:TYR:CD2	1:A:200:TYR:C	2.89	0.45
1:C:98:LEU:HA	1:C:225:TRP:CZ3	2.49	0.45
1:E:192:LEU:N	1:E:239:ASN:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:CYS:HB2	1:C:278:THR:HG21	1.98	0.45
1:E:186:TYR:CZ	1:E:241:ALA:HA	2.52	0.45
1:A:186:TYR:CZ	1:A:241:ALA:HA	2.51	0.45
2:F:77:ILE:HA	2:F:77:ILE:HD12	1.78	0.45
2:B:52:LEU:HA	2:B:52:LEU:HD12	1.84	0.45
1:E:213:GLN:HA	1:E:217:GLN:O	2.15	0.45
1:A:192:LEU:HD22	1:A:193:ILE:H	1.81	0.45
2:B:26:HIS:HB2	2:B:149:MET:HE2	1.99	0.45
1:C:5:LEU:HD22	1:C:5:LEU:N	2.12	0.44
1:A:5:LEU:HD21	2:B:119:TYR:HD1	1.82	0.44
1:E:99:ARG:O	1:E:103:ARG:HG3	2.17	0.44
1:C:165:ASP:HB3	1:C:166:PRO:CD	2.48	0.44
2:F:150:ALA:O	2:F:154:ASN:ND2	2.50	0.44
1:A:165:ASP:HB3	1:A:166:PRO:CD	2.48	0.44
1:A:57:LEU:HD21	1:A:99:ARG:HG2	2.00	0.44
1:E:165:ASP:HB3	1:E:166:PRO:CD	2.48	0.44
1:E:230:PRO:O	1:E:231:ASN:HB2	2.17	0.44
1:A:291:ARG:HH12	2:B:67:ASP:HB3	1.82	0.44
2:F:26:HIS:ND1	2:F:26:HIS:C	2.71	0.44
1:A:230:PRO:O	1:A:231:ASN:HB2	2.18	0.44
1:A:103:ARG:HB3	1:A:257:GLY:HA3	1.99	0.43
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.99	0.43
1:C:200:TYR:C	1:C:200:TYR:CD2	2.91	0.43
2:D:26:HIS:HB2	2:D:149:MET:HE2	2.00	0.43
1:E:152:PHE:HA	1:E:153:PRO:HD3	1.87	0.43
1:E:200:TYR:CD2	1:E:200:TYR:C	2.90	0.43
1:A:120:ILE:HG23	1:A:145:SER:HA	2.01	0.43
1:A:207:SER:O	1:A:211:ARG:NH2	2.46	0.43
1:A:226:LEU:C	1:A:226:LEU:HD12	2.39	0.43
1:E:1:ASP:HB2	2:F:27:GLN:O	2.19	0.43
1:E:88:TYR:CD2	1:E:221:ILE:HD12	2.53	0.43
1:E:226:LEU:C	1:E:226:LEU:HD12	2.38	0.43
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.99	0.43
1:A:232:ASP:OD2	1:A:233:THR:N	2.49	0.43
1:E:92:PHE:CE2	1:E:170:ILE:HD11	2.44	0.43
1:E:41:ILE:HD11	1:E:260:SER:CB	2.49	0.43
1:A:213:GLN:OE1	1:A:216:GLY:HA2	2.19	0.43
2:B:25:ARG:NE	2:B:34:THR:CG2	2.66	0.43
1:A:191:LYS:HE3	1:A:191:LYS:HB3	1.88	0.43
2:D:88:MET:HB3	2:D:88:MET:HE2	1.88	0.43
2:D:25:ARG:NE	2:D:34:THR:HG21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:GLN:OE1	2:F:90:GLU:HG2	2.19	0.42
2:D:67:ASP:OD2	2:D:85:ARG:NH2	2.50	0.42
2:F:107:THR:HA	2:F:110:LEU:HD13	2.01	0.42
2:B:26:HIS:C	2:B:26:HIS:ND1	2.73	0.42
1:C:5:LEU:HD21	2:D:119:TYR:HD1	1.83	0.42
2:D:52:LEU:HD12	2:D:52:LEU:HA	1.84	0.42
1:E:232:ASP:OD2	1:E:233:THR:N	2.49	0.42
1:A:32:THR:HB	1:A:305:LEU:O	2.20	0.42
1:E:90:GLY:HA3	1:E:221:ILE:O	2.19	0.42
2:D:57:GLU:OE1	2:D:57:GLU:N	2.53	0.42
1:C:230:PRO:O	1:C:231:ASN:HB2	2.20	0.42
1:E:163:ARG:HD3	1:E:250:PHE:CZ	2.54	0.42
1:E:265:ASP:OD2	1:E:268:CYS:SG	2.78	0.42
1:A:56:LEU:O	1:A:59:THR:HB	2.19	0.42
2:F:26:HIS:HB2	2:F:149:MET:HE2	2.01	0.42
2:B:48:ILE:HD11	2:B:107:THR:HG23	2.02	0.42
2:D:107:THR:HA	2:D:110:LEU:HD13	2.02	0.42
2:F:57:GLU:CG	2:F:58:LYS:N	2.77	0.42
2:D:26:HIS:C	2:D:26:HIS:ND1	2.74	0.41
1:E:120:ILE:HG23	1:E:145:SER:HA	2.01	0.41
1:E:147:THR:CG2	1:E:148:ASP:N	2.83	0.41
1:C:192:LEU:N	1:C:239:ASN:OD1	2.50	0.41
1:A:164:LYS:HB2	1:A:164:LYS:HE3	1.75	0.41
2:D:150:ALA:O	2:D:154:ASN:ND2	2.54	0.41
2:F:122:VAL:O	2:F:123:LYS:C	2.59	0.41
1:A:181:GLU:OE1	1:A:181:GLU:HA	2.21	0.41
1:A:235:THR:HG22	1:C:212:PRO:HG3	2.02	0.41
2:B:129:ASN:OD1	2:B:129:ASN:N	2.53	0.41
1:A:192:LEU:N	1:A:239:ASN:OD1	2.53	0.41
1:E:314:VAL:HA	1:E:315:PRO:HD3	1.84	0.41
2:F:158:ASP:OD2	2:F:161:LYS:HB2	2.20	0.41
2:F:25:ARG:NE	2:F:34:THR:HG21	2.35	0.41
2:B:57:GLU:OE1	2:B:57:GLU:N	2.53	0.41
2:B:77:ILE:HD12	2:B:77:ILE:HA	1.80	0.41
1:E:31:GLU:HG3	1:E:32:THR:N	2.35	0.41
1:E:181:GLU:HA	1:E:181:GLU:OE1	2.20	0.41
2:F:57:GLU:N	2:F:57:GLU:OE1	2.54	0.41
2:F:88:MET:HE2	2:F:88:MET:HB3	1.85	0.41
1:A:1:ASP:HB2	2:B:27:GLN:O	2.21	0.41
1:C:291:ARG:HH12	2:D:67:ASP:HB3	1.83	0.41
1:A:32:THR:HG23	1:A:285:PHE:HD1	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:ILE:N	2:B:10:ILE:HD12	2.36	0.40
1:E:5:LEU:HD21	2:F:119:TYR:HD1	1.86	0.40
1:E:5:LEU:HD22	1:E:5:LEU:N	2.13	0.40
2:F:159:HIS:CG	2:F:160:SER:N	2.89	0.40
1:A:123:ASN:O	1:A:125:THR:HG23	2.21	0.40
1:C:41:ILE:HD11	1:C:260:SER:CB	2.51	0.40
2:D:77:ILE:HD12	2:D:77:ILE:HA	1.75	0.40
2:B:159:HIS:CG	2:B:160:SER:N	2.89	0.40
1:A:212:PRO:HG3	1:E:235:THR:HG22	2.03	0.40
2:F:126:LEU:O	2:F:127:ARG:C	2.60	0.40
1:C:152:PHE:HA	1:C:153:PRO:HD3	1.86	0.40
1:C:81:ARG:NH1	1:C:261:GLU:OE2	2.53	0.40
1:C:314:VAL:HA	1:C:315:PRO:HD3	1.83	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	314/327 (96%)	287 (91%)	26 (8%)	1 (0%)	41	72
1	C	314/327 (96%)	285 (91%)	28 (9%)	1 (0%)	41	72
1	E	316/327 (97%)	288 (91%)	26 (8%)	2 (1%)	25	56
2	B	168/177 (95%)	158 (94%)	9 (5%)	1 (1%)	25	56
2	D	169/177 (96%)	157 (93%)	11 (6%)	1 (1%)	25	56
2	F	167/177 (94%)	155 (93%)	11 (7%)	1 (1%)	25	56
All	All	1448/1512 (96%)	1330 (92%)	111 (8%)	7 (0%)	29	61

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	127	ARG
1	C	148	ASP
1	A	148	ASP
2	B	127	ARG
1	E	150	ALA
2	F	127	ARG
1	E	52	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	268/277 (97%)	236 (88%)	32 (12%)	5 16
1	C	268/277 (97%)	234 (87%)	34 (13%)	4 14
1	E	269/277 (97%)	235 (87%)	34 (13%)	4 14
2	B	145/151 (96%)	131 (90%)	14 (10%)	8 24
2	D	146/151 (97%)	129 (88%)	17 (12%)	5 17
2	F	144/151 (95%)	128 (89%)	16 (11%)	6 19
All	All	1240/1284 (97%)	1093 (88%)	147 (12%)	5 16

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	8	HIS
1	A	14	THR
1	A	20	THR
1	A	24	VAL
1	A	32	THR
1	A	59	THR
1	A	65	GLN
1	A	73	SER
1	A	82	GLU
1	A	86	VAL
1	A	121	ARG

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Mol	Chain	Res	Type
1	A	122	THR
1	A	126	THR
1	A	143	LEU
1	A	162	THR
1	A	165	ASP
1	A	170	ILE
1	A	176	SER
1	A	178	SER
1	A	180	THR
1	A	182	GLN
1	A	192	LEU
1	A	194	THR
1	A	200	TYR
1	A	203	SER
1	A	207	SER
1	A	217	GLN
1	A	235	THR
1	A	261	GLU
1	A	263	GLN
1	A	298	ARG
2	B	11	GLU
2	B	26	HIS
2	B	32	GLU
2	B	48	ILE
2	B	52	LEU
2	B	57	GLU
2	B	59	THR
2	B	66	ILE
2	B	72	GLU
2	B	110	LEU
2	B	115	MET
2	B	129	ASN
2	B	133	ASP
2	B	149	MET
1	C	5	LEU
1	C	8	HIS
1	C	14	THR
1	C	20	THR
1	C	24	VAL
1	C	32	THR
1	C	59	THR
1	C	65	GLN

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Mol	Chain	Res	Type
1	C	73	SER
1	C	82	GLU
1	C	86	VAL
1	C	121	ARG
1	C	122	THR
1	C	126	THR
1	C	129	CYS
1	C	143	LEU
1	C	165	ASP
1	C	170	ILE
1	C	176	SER
1	C	178	SER
1	C	182	GLN
1	C	194	THR
1	C	200	TYR
1	C	203	SER
1	C	205	VAL
1	C	217	GLN
1	C	225	TRP
1	C	235	THR
1	C	251	LEU
1	C	261	GLU
1	C	263	GLN
1	C	291	ARG
1	C	298	ARG
1	C	312	LYS
2	D	11	GLU
2	D	26	HIS
2	D	32	GLU
2	D	39	LYS
2	D	48	ILE
2	D	52	LEU
2	D	57	GLU
2	D	59	THR
2	D	66	ILE
2	D	72	GLU
2	D	110	LEU
2	D	115	MET
2	D	121	ARG
2	D	129	ASN
2	D	133	ASP
2	D	149	MET

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Mol	Chain	Res	Type
2	D	171	ILE
1	E	5	LEU
1	E	8	HIS
1	E	14	THR
1	E	20	THR
1	E	24	VAL
1	E	32	THR
1	E	59	THR
1	E	65	GLN
1	E	73	SER
1	E	82	GLU
1	E	86	VAL
1	E	121	ARG
1	E	122	THR
1	E	126	THR
1	E	129	CYS
1	E	143	LEU
1	E	148	ASP
1	E	164	LYS
1	E	165	ASP
1	E	170	ILE
1	E	176	SER
1	E	178	SER
1	E	180	THR
1	E	182	GLN
1	E	192	LEU
1	E	194	THR
1	E	200	TYR
1	E	203	SER
1	E	207	SER
1	E	217	GLN
1	E	263	GLN
1	E	291	ARG
1	E	298	ARG
1	E	312	LYS
2	F	11	GLU
2	F	26	HIS
2	F	32	GLU
2	F	39	LYS
2	F	48	ILE
2	F	52	LEU
2	F	57	GLU

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Mol	Chain	Res	Type
2	F	59	THR
2	F	66	ILE
2	F	72	GLU
2	F	110	LEU
2	F	115	MET
2	F	129	ASN
2	F	133	ASP
2	F	149	MET
2	F	169	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	403	1	14,14,15	0.56	0	17,19,21	1.57	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SIA	A	404	-	17,20,21	1.09	1 (5%)	21,28,31	1.91	4 (19%)
3	NAG	A	403	1	14,14,15	0.66	0	17,19,21	1.95	4 (23%)
3	NAG	F	201	2	14,14,15	0.70	0	17,19,21	1.82	4 (23%)
4	SIA	C	404	-	17,20,21	1.12	1 (5%)	21,28,31	2.14	7 (33%)
3	NAG	D	201	2	14,14,15	0.57	0	17,19,21	2.05	6 (35%)
3	NAG	A	401	1	14,14,15	0.47	0	17,19,21	1.11	1 (5%)
3	NAG	B	201	2	14,14,15	0.59	0	17,19,21	2.18	5 (29%)
3	NAG	E	401	1	14,14,15	0.65	0	17,19,21	1.49	3 (17%)
4	SIA	E	404	-	17,20,21	1.17	1 (5%)	21,28,31	1.91	6 (28%)
3	NAG	C	402	1	14,14,15	0.54	0	17,19,21	2.28	4 (23%)
3	NAG	A	402	1	14,14,15	0.52	0	17,19,21	2.53	5 (29%)
3	NAG	C	401	1	14,14,15	0.50	0	17,19,21	2.11	4 (23%)
3	NAG	E	402	1	14,14,15	0.53	0	17,19,21	2.22	3 (17%)
3	NAG	E	403	1	14,14,15	0.50	0	17,19,21	1.21	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	403	1	-	2/6/23/26	0/1/1/1
4	SIA	A	404	-	-	4/14/34/38	0/1/1/1
3	NAG	A	403	1	-	3/6/23/26	0/1/1/1
3	NAG	F	201	2	-	0/6/23/26	0/1/1/1
4	SIA	C	404	-	-	4/14/34/38	0/1/1/1
3	NAG	D	201	2	-	0/6/23/26	0/1/1/1
3	NAG	A	401	1	-	1/6/23/26	0/1/1/1
3	NAG	B	201	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	1	-	1/6/23/26	0/1/1/1
4	SIA	E	404	-	-	4/14/34/38	0/1/1/1
3	NAG	C	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	C	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	402	1	-	0/6/23/26	0/1/1/1
3	NAG	E	403	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	404	SIA	C7-C6	3.27	1.57	1.53
4	A	404	SIA	C7-C6	3.17	1.57	1.53
4	C	404	SIA	C7-C6	2.85	1.56	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	NAG	C1-O5-C5	7.50	122.35	112.19
3	E	402	NAG	C1-O5-C5	7.19	121.94	112.19
3	C	402	NAG	C1-O5-C5	7.00	121.68	112.19
3	B	201	NAG	C1-O5-C5	6.52	121.03	112.19
3	D	201	NAG	C1-O5-C5	5.21	119.26	112.19
3	A	403	NAG	C1-O5-C5	5.20	119.24	112.19
3	C	401	NAG	C1-C2-N2	-4.82	102.26	110.49
4	A	404	SIA	C6-O6-C2	4.74	121.47	111.34
4	E	404	SIA	C6-O6-C2	4.67	121.33	111.34
4	C	404	SIA	C6-O6-C2	4.58	121.14	111.34
3	C	401	NAG	C1-O5-C5	4.52	118.32	112.19
4	A	404	SIA	C8-C7-C6	4.13	120.87	113.03
4	C	404	SIA	C8-C7-C6	4.08	120.77	113.03
4	E	404	SIA	C8-C7-C6	3.91	120.44	113.03
3	A	402	NAG	O3-C3-C2	-3.82	101.57	109.47
3	A	403	NAG	C1-C2-N2	3.77	116.92	110.49
3	E	401	NAG	C1-O5-C5	3.75	117.27	112.19
4	C	404	SIA	C3-C4-C5	-3.71	106.97	111.46
3	A	402	NAG	O5-C1-C2	3.64	117.04	111.29
3	F	201	NAG	C1-O5-C5	3.60	117.07	112.19
3	F	201	NAG	C2-N2-C7	3.50	127.89	122.90
3	A	401	NAG	C1-O5-C5	3.38	116.78	112.19
3	A	403	NAG	O5-C1-C2	-3.26	106.14	111.29
4	A	404	SIA	C3-C4-C5	-3.24	107.54	111.46
3	E	401	NAG	C1-C2-N2	-3.23	104.97	110.49
4	C	404	SIA	O6-C2-C3	3.22	115.52	109.87
3	C	401	NAG	O5-C1-C2	3.21	116.35	111.29
3	C	402	NAG	O3-C3-C2	-3.12	103.02	109.47
3	C	401	NAG	O5-C5-C6	3.10	112.06	107.20
3	E	403	NAG	C1-O5-C5	3.09	116.38	112.19
3	C	403	NAG	C1-O5-C5	3.06	116.34	112.19
3	C	403	NAG	O5-C1-C2	-3.06	106.45	111.29
3	D	201	NAG	C2-N2-C7	2.90	127.03	122.90
4	E	404	SIA	O6-C2-C3	2.82	114.82	109.87
4	C	404	SIA	O9-C9-C8	2.82	117.21	111.07
3	C	403	NAG	O5-C5-C6	2.79	111.58	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	404	SIA	C11-C10-N5	2.74	120.74	116.10
3	E	402	NAG	O3-C3-C2	-2.66	103.96	109.47
3	A	402	NAG	C2-N2-C7	-2.66	119.11	122.90
3	C	402	NAG	C6-C5-C4	-2.59	106.93	113.00
3	F	201	NAG	O7-C7-N2	2.59	126.72	121.95
3	B	201	NAG	O4-C4-C3	2.58	116.31	110.35
3	B	201	NAG	O3-C3-C4	2.53	116.19	110.35
4	E	404	SIA	C3-C4-C5	-2.50	108.43	111.46
3	D	201	NAG	O3-C3-C4	2.50	116.12	110.35
3	F	201	NAG	O4-C4-C3	2.49	116.10	110.35
4	E	404	SIA	C11-C10-N5	2.46	120.26	116.10
3	B	201	NAG	C8-C7-N2	-2.42	112.00	116.10
4	E	404	SIA	O9-C9-C8	2.37	116.24	111.07
3	E	402	NAG	C2-N2-C7	-2.34	119.57	122.90
3	C	402	NAG	O5-C1-C2	2.30	114.92	111.29
3	D	201	NAG	O7-C7-N2	2.30	126.18	121.95
3	A	402	NAG	C6-C5-C4	-2.30	107.62	113.00
4	C	404	SIA	O4-C4-C5	2.27	115.00	109.77
4	A	404	SIA	C11-C10-N5	2.27	119.94	116.10
3	A	403	NAG	O5-C5-C6	2.17	110.60	107.20
3	B	201	NAG	O7-C7-N2	2.17	125.94	121.95
3	C	403	NAG	O7-C7-C8	-2.11	118.14	122.06
3	E	401	NAG	C4-C3-C2	2.10	114.09	111.02
3	D	201	NAG	C4-C3-C2	-2.08	107.97	111.02
3	D	201	NAG	O4-C4-C3	2.04	115.07	110.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	404	SIA	O8-C8-C9-O9
4	A	404	SIA	C11-C10-N5-C5
4	A	404	SIA	O10-C10-N5-C5
4	C	404	SIA	C7-C8-C9-O9
4	C	404	SIA	O8-C8-C9-O9
4	C	404	SIA	C11-C10-N5-C5
3	C	403	NAG	O5-C5-C6-O6
3	A	403	NAG	O5-C5-C6-O6
3	E	403	NAG	O5-C5-C6-O6
3	C	401	NAG	O5-C5-C6-O6
4	A	404	SIA	C7-C8-C9-O9
3	C	401	NAG	C4-C5-C6-O6

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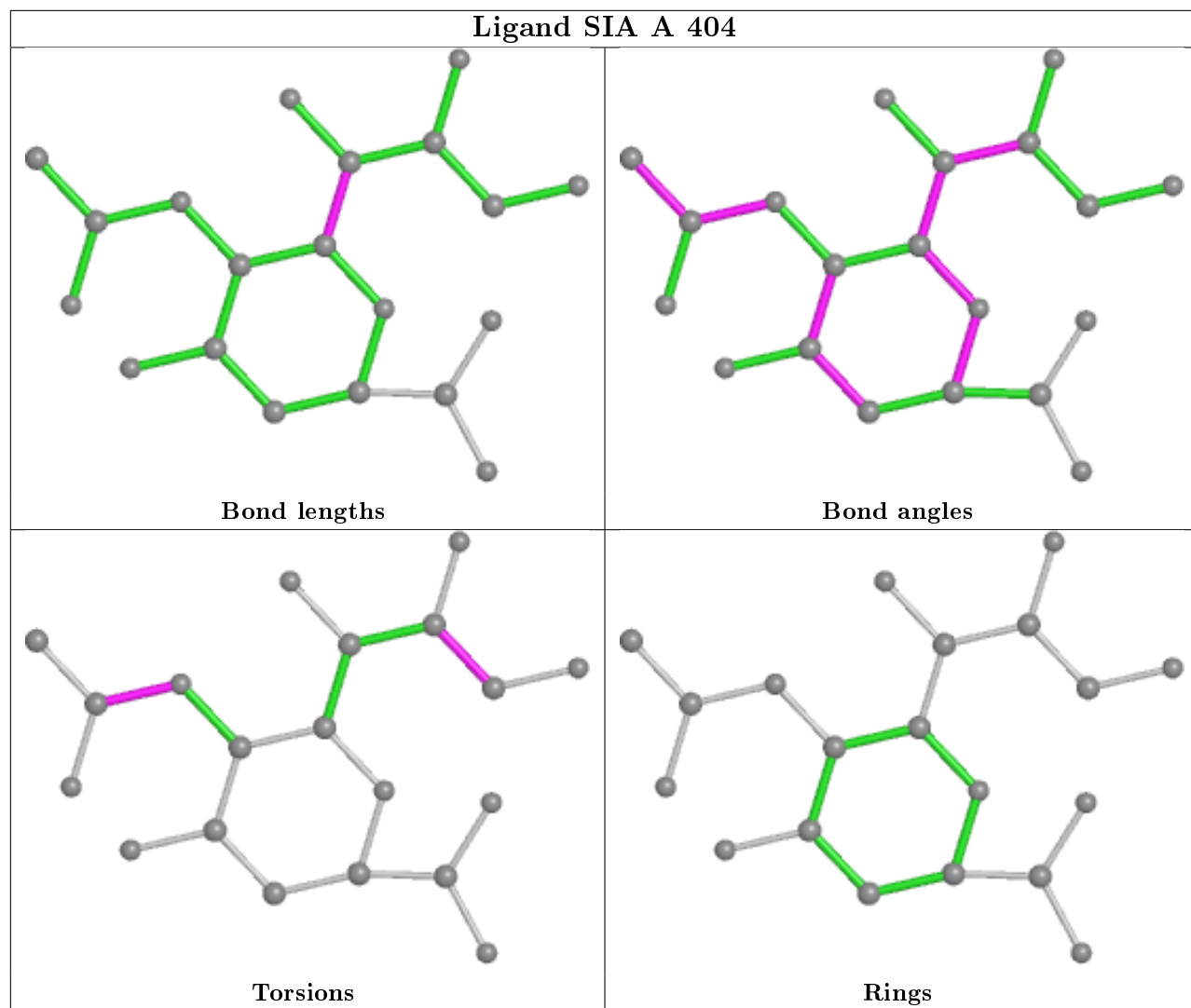
Mol	Chain	Res	Type	Atoms
4	C	404	SIA	O10-C10-N5-C5
3	A	403	NAG	C4-C5-C6-O6
3	E	403	NAG	C4-C5-C6-O6
3	C	403	NAG	C4-C5-C6-O6
4	E	404	SIA	C11-C10-N5-C5
4	E	404	SIA	O10-C10-N5-C5
4	E	404	SIA	C7-C8-C9-O9
3	A	401	NAG	O5-C5-C6-O6
4	E	404	SIA	O8-C8-C9-O9
3	A	403	NAG	C3-C2-N2-C7
3	E	401	NAG	O5-C5-C6-O6

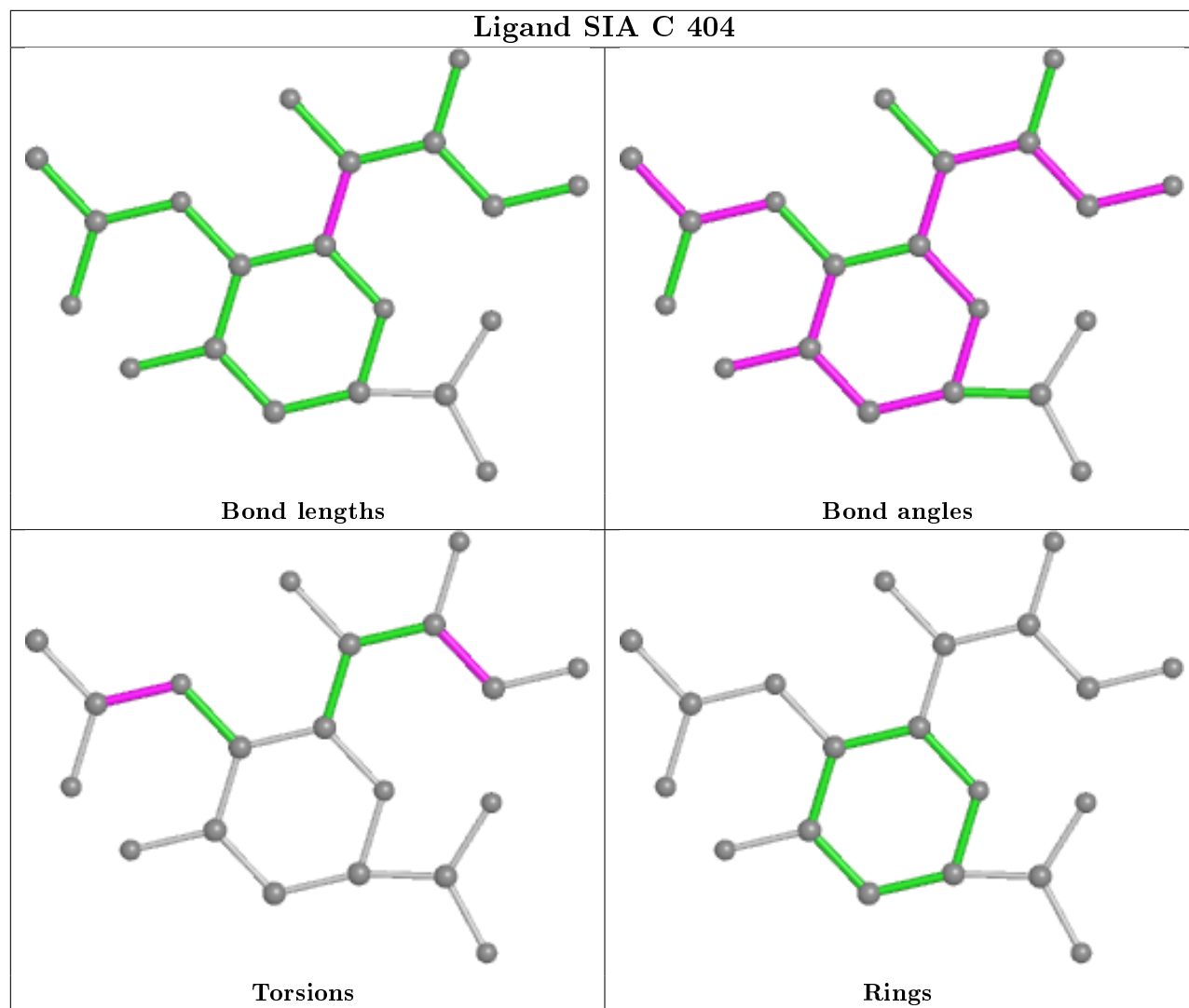
There are no ring outliers.

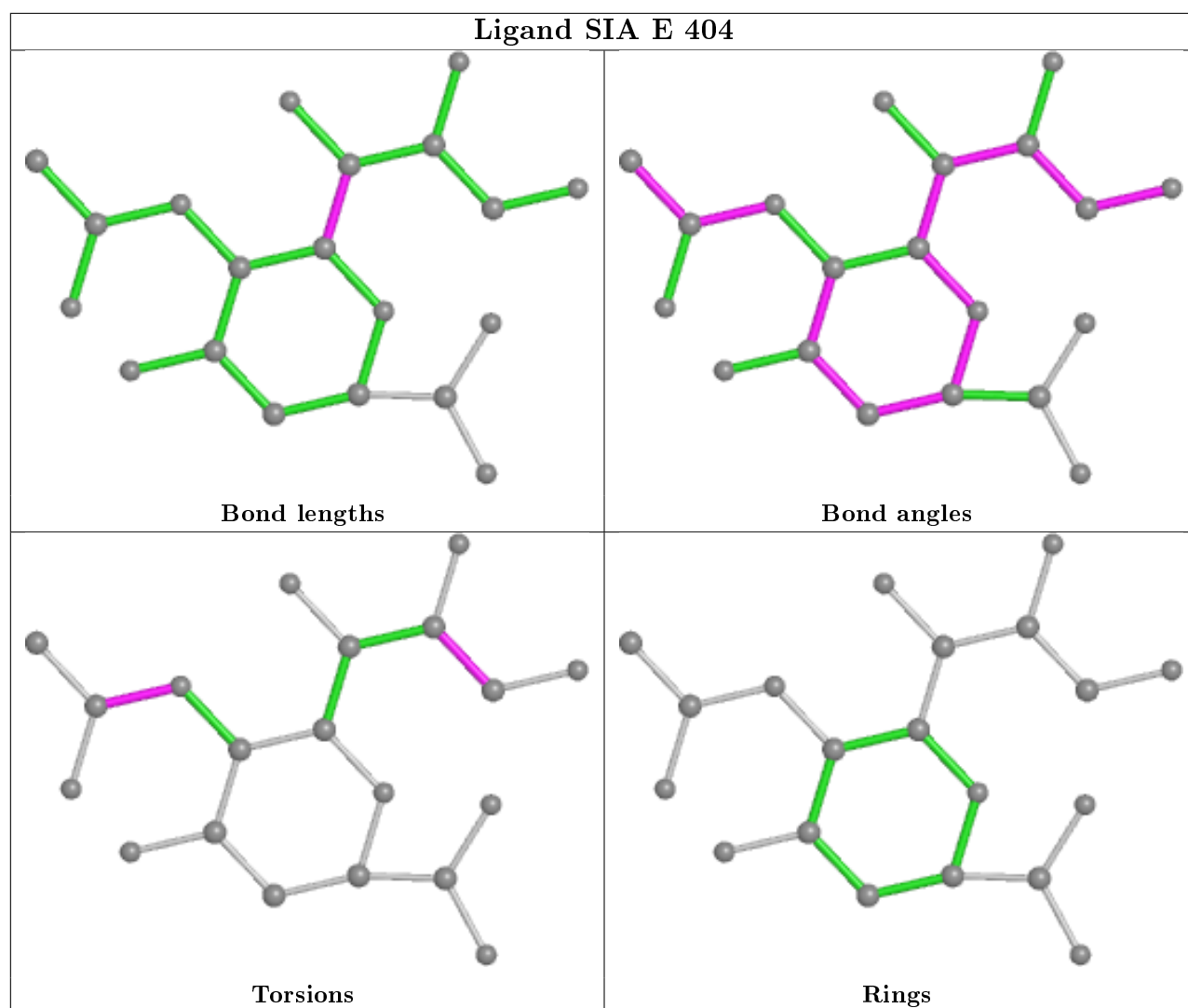
2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	201	NAG	2	0
3	D	201	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	316/327 (96%)	-0.37	0 100 100	19, 46, 88, 114	1 (0%)
1	C	316/327 (96%)	-0.33	1 (0%) 94 93	19, 47, 89, 112	3 (0%)
1	E	317/327 (96%)	-0.36	0 100 100	20, 45, 86, 115	2 (0%)
2	B	170/177 (96%)	-0.29	2 (1%) 79 73	17, 64, 107, 118	1 (0%)
2	D	171/177 (96%)	-0.28	3 (1%) 68 61	17, 64, 106, 118	0
2	F	169/177 (95%)	-0.30	1 (0%) 89 86	18, 62, 108, 113	0
All	All	1459/1512 (96%)	-0.33	7 (0%) 91 88	17, 52, 98, 118	7 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	198	SER	3.2
2	D	60	ASN	2.3
2	D	168	GLN	2.3
2	B	167	ILE	2.3
2	D	3	PHE	2.2
2	F	60	ASN	2.2
2	B	60	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

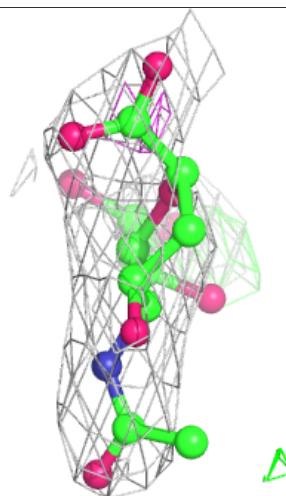
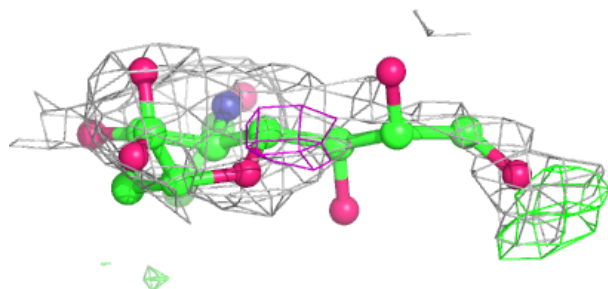
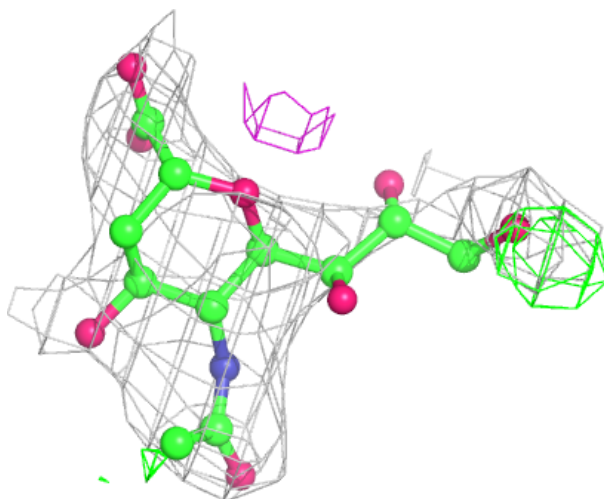
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	A	403	14/15	0.77	0.22	92,129,157,166	0
4	SIA	C	404	20/21	0.80	0.38	111,138,176,195	0
3	NAG	C	403	14/15	0.81	0.18	103,126,148,157	0
4	SIA	A	404	20/21	0.82	0.41	119,147,190,237	0
3	NAG	A	402	14/15	0.82	0.17	76,118,143,150	0
3	NAG	E	403	14/15	0.82	0.18	96,128,156,157	0
3	NAG	C	401	14/15	0.84	0.21	98,123,145,154	0
4	SIA	E	404	20/21	0.84	0.43	99,130,177,200	0
3	NAG	C	402	14/15	0.87	0.16	83,114,141,143	0
3	NAG	E	401	14/15	0.88	0.16	94,114,131,138	0
3	NAG	A	401	14/15	0.89	0.16	103,123,143,145	0
3	NAG	E	402	14/15	0.90	0.16	84,121,148,151	0
3	NAG	D	201	14/15	0.90	0.14	61,83,94,97	0
3	NAG	B	201	14/15	0.91	0.14	57,74,98,107	0
3	NAG	F	201	14/15	0.92	0.14	58,80,95,101	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

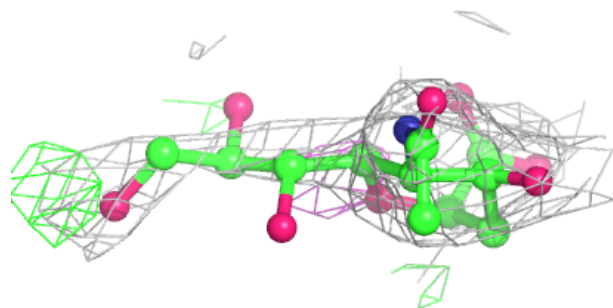
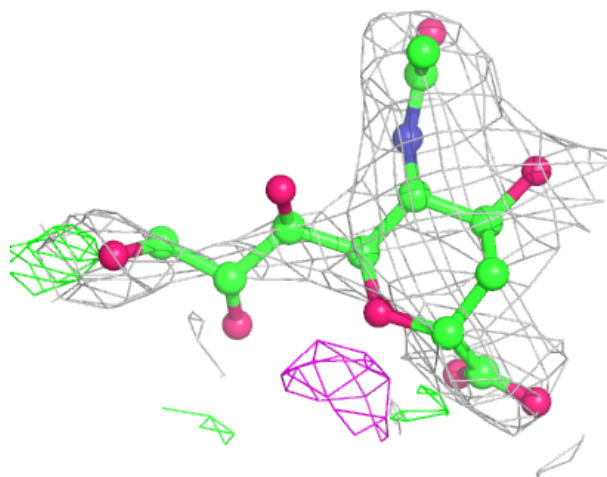
Electron density around SIA C 404:

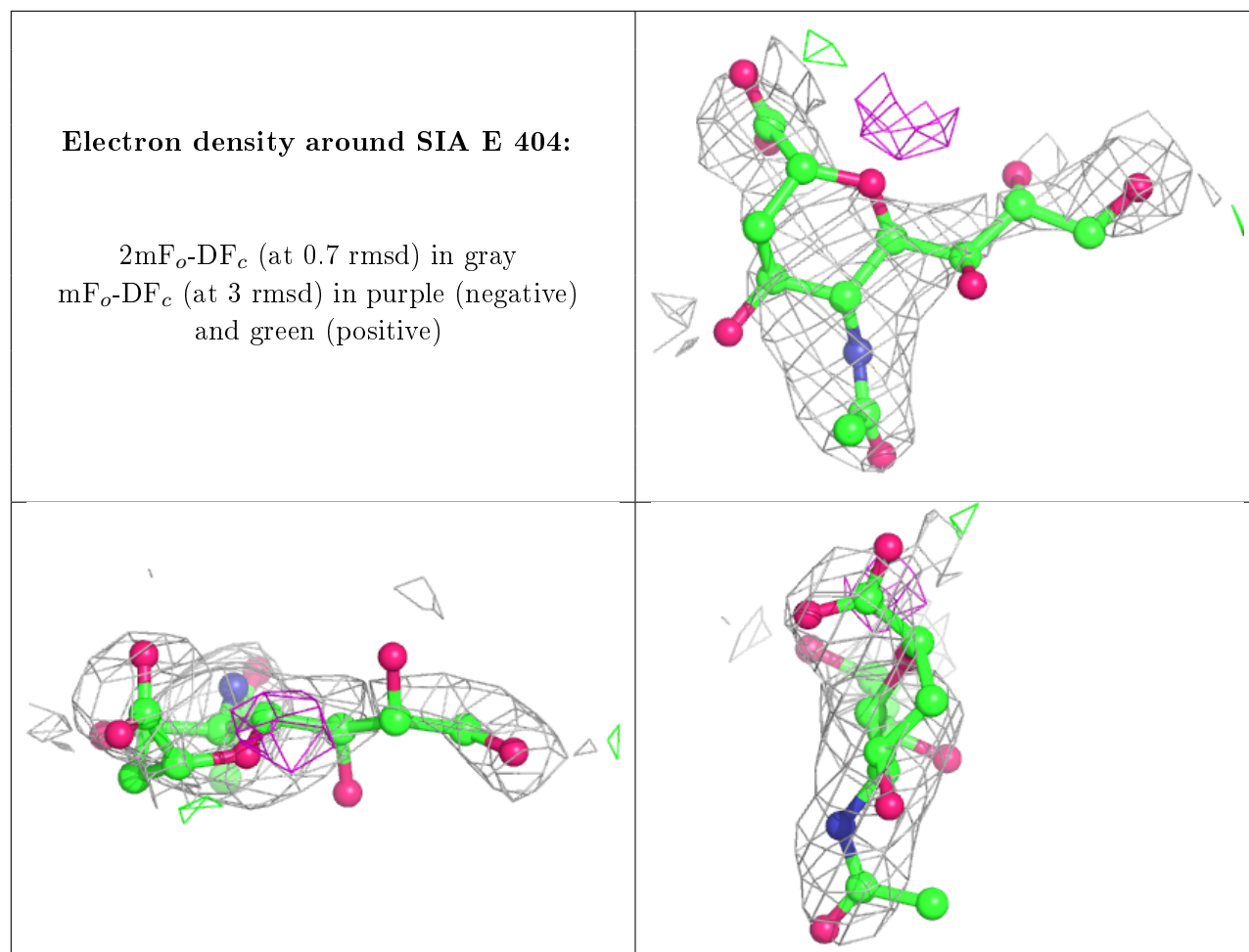
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SIA A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.